Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.93e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.64e-01

Confidence level: 5.91e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
1,5-Dihydroxynaphthalene	1,3-Naphthalenediol	2,2-Bis(bromomethyl)-1,3-propanediol
Measured: 1.03e-03	**Measured:** 1.12e-02	**Measured:** 1.45e-01
Predicted: 8.87e-03	**Predicted:** 2.01e-02	**Predicted:** 2.34e-01